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## Journal of Power Sources Advances



journal homepage: www.journals.elsevier.com/journal-of-power-sources-advances

# Numerical simulation of mass transfer enhancement in liquid metal batteries by means of electro-vortex flow



Norbert Weber<sup>a,\*</sup>, Michael Nimtz<sup>a</sup>, Paolo Personnettaz<sup>a</sup>, Tom Weier<sup>a</sup>, Donald Sadoway<sup>b</sup>

<sup>a</sup> Helmholtz-Zentrum Dresden – Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

<sup>b</sup> Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, 02139-4307, United States

ARTICLE INFO	A B S T R A C T				
Keywords: Liquid metal battery Concentration polarisation Electro-vortex flow Mixing Mass transfer enhancement	Mass transfer is of paramount importance for an efficient operation of liquid metal batteries. We show for the first time that electrodynamically driven flow can indeed improve mixing of liquid electrodes, and reduces concentration polarisation substantially. Simulating the discharge of a realistic Li  Bi cell at 1 A/cm <sup>2</sup> , the corresponding overpotential reduces by up to 62%. Moreover, the formation of intermetallic phases is delayed, which improves capacity usage. Finally, we demonstrate that vertical magnetic fields – which are originating from external sources.				
	- change the flow structure entirely, and will homogenise the positive electrode even better.				

### 1. Introduction

Liquid metal batteries (LMBs) consist of two liquid metal electrodes, which are separated by a molten salt electrolyte. The three phases selfsegregate due to mutual immiscibility, as illustrated in Fig. 1. When discharging such cells, the anode metal is transferred from the negative to the positive electrode, where it alloys with the cathode metal. Employing earth-abundant elements, LMBs are ideal candidates for low-cost stationary energy storage with a long lifetime and high current densities [1]. They are perfectly suited for applications like load levelling or frequency control, and will help to include intermittent renewable energies into the electric grid.

Almost 60 years ago, Agruss et al. [3] noticed that this alloying is a slow process. Especially at elevated currents, a thin layer with a high concentration of the anode metal develops on top of the positive electrode. As the cell potential depends directly on the interface concentration, it decreases. Such polarisation effects were observed later in many different Na and K-based LMBs [4–7], but especially at high discharge currents [8]. Similarly, anode-metal-depleted layers were observed during charge of the cells [7]. Finally, it was also noticed that mass transfer in the positive electrode determines the maximum charge and discharge current of a cell [9,10].

As soon as the anode metal exceeds locally a certain concentration, a solid intermetallic forms [10,11]. These intermetallic phases are typically of low density, and therefore float on top of the positive electrode [12]. Dendrites may even grow through the electrolyte and short-circuit the cell

[13,14]. While intermetallic layers are generally detrimental to the operation of Na-, K- and Ca-based cells, Li||Bi LMBs can perfectly be operated even with an intermetallic layer [2], because diffusion of Li in the Li<sub>3</sub>Bi phase is only an order of magnitude slower than in the liquid alloy.

Already in the early days it was noticed that convectional stirring of the positive electrode might prevent the formation of concentration layers [7], and increase the performance of LMBs. Mixing effects due to surface tension gradients were expected to appear naturally [3], but also thermal convection [10] and even mechanical stirring for reducing concentration effects were discussed in the 1960s [6,11].

Unfortunately, the stratification in the concentration layers is typically strong because of the large density difference between anode and cathode metal [15]. Consequently, it is not easy to generate a sufficiently violent fluid flow that is able to mix the positive electrode. For example, thermal convection is comparably weak and will not drive a substantial flow in the positive electrode during normal operation of the cells [16–18] – only a strong external heating from the side or the bottom might be used for that purpose [19–21]. Still, the mixing effect is assumed to be small.

Fortunately, concentration polarisation is negligible when charging an LMB. There, strong solutal convection develops, and mixes the alloy thoroughly [22]. The missing brick is, therefore, a means to drive flow during discharge. For this purpose, electro-vortex flow was often discussed to be useful [23,24]. Such electrodynamically driven flow appears where current lines diverge [25], and will therefore always be present in LMBs [26–28].

\* Corresponding author. *E-mail address:* norbert.weber@hzdr.de (N. Weber).

https://doi.org/10.1016/j.powera.2020.100004

Received 4 January 2020; Received in revised form 11 February 2020; Accepted 13 February 2020

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Fig. 1. Setup and dimensions of the studied cell. The battery is cylindrical, and the dimensions are in mm [2].

We will show in this article for the first time that electro-vortex flow is indeed strong enough to counteract the stable stratification and to reduce the concentration gradient thickness in a realistic battery, thereby increasing cell voltage and efficiency, and delaying the formation of local intermetallics. All simulations are done for a fully three-dimensional LMB, with a realistic aspect ratio of the positive electrode and with realistic boundary conditions at the fluid-fluid interface.

#### 2. Physical and numerical model

#### 2.1. Liquid metal battery experiment & material properties

We model a Li||Bi cell, which was experimentally studied by Ning et al. [2] - Fig. 1 gives the dimensions. As a simplification, we always assume the metal foam to be fully filled with Li. Moreover, we take the thickness of the positive electrode as constant (2.8 mm), corresponding to a fully charged cell.

The battery is operated at 550°C; the corresponding material properties are given in Table 1. As a simplification we use the transport properties of Bi for the alloy, as well. The solutal expansion coefficient is estimated as  $\beta = 1.3 \cdot 10^{-3} \text{ m}^3/\text{kg}$  for a molar fraction of Li in Bi up to 0.525 using Vegard's law. The diffusion coefficient of Li in Bi is assumed to be constant in the whole concentration range, and is estimated as  $D = 8 \cdot 10^{-9} \text{ m}^2/\text{s}$  [29]. Finally, the open circuit potential is fitted for 550°C with data from Gasior [30] as

$$E_{\rm ocv} = 0.71 - 0.078 \cdot \ln(x) - 0.029x - 0.27x^2.$$
<sup>(1)</sup>

At molar fractions larger than x = 0.525 the intermetallic phase forms and the open circuit potential stays constant as  $E_{oev} = 0.663$  V.

#### 2.2. Numerical model

We use a fully three-dimensional model implemented in the open source CFD library OpenFOAM [37]. Employing the parent-child mesh method [38], we create one global mesh for the complete battery, as well as two separate meshes, one for the cathode and one for the electrolyte. While a solution for certain variables (e.g. current density) is computed on the global mesh, other variables (e.g. flow velocity) are solved for only on the child meshes. As the meshes are perfectly overlapping, variables can easily be mapped between them.

Applying a constant current at both electrodes, we solve the electric potential  $\varphi$  in the entire battery in a first step as

$$\nabla \cdot \sigma \nabla \varphi = 0, \tag{2}$$

with  $\sigma$  denoting the electric conductivity. We create the matrix for the Poisson equation in such a way that the electric potential at the interface between electrolyte and positive electrode increases stepwise by the magnitude of the open circuit potential (eqn. (1)). As no current can flow from the electrolyte to the housing, we decouple the potential at this interface. Thereafter, we find the current density as

$$j = -\sigma \nabla \varphi. \tag{3}$$

The magnetic field inside the LMB is determined by solving the induction equation in the quasi-static limit [38,39]

$$0 = \Delta \boldsymbol{b},\tag{4}$$

with the boundary condition obtained from Biot-Savart's law as

$$\boldsymbol{b}(\boldsymbol{r}) = \frac{\mu_0}{4\pi} \int \frac{\boldsymbol{j}(\boldsymbol{r}') \times (\boldsymbol{r} - \boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|^3} dV'.$$
(5)

This gives finally the Lorentz force

$$\boldsymbol{f} = \boldsymbol{j} \times \boldsymbol{b}. \tag{6}$$

Using the inductionless approximation, we assume the Lorentz force to be constant during the simulation [38]. This is justified as the magnetic Reynolds number of the alloy  $Rm \approx 10^{-4}$  is considerably lower than 0.01.

We map the computed Lorentz force to two separate fluid meshes for the positive electrode and the electrolyte. There, we solve the Navier-Stokes equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) = -\nabla p_d + \nabla \cdot (\nu \nabla \boldsymbol{u}) - \boldsymbol{g} \cdot \boldsymbol{x} \nabla \rho_k + \frac{\boldsymbol{f}}{\rho_0}$$
(7)

$$\nabla \cdot \boldsymbol{u} = \boldsymbol{0},\tag{8}$$

with *u* denoting velocity, *t* time, *g* gravity, *x* the coordinate vector,  $p_d$  a modified pressure [40],  $\nu$  the kinematic viscosity and  $\rho_0$  the reference density, which is obtained using Vegard's law. Using the Oberbeck-Boussinesq approximation, we account for density changes only in the gravity term and compute the relative density change as

$$\rho_k = 1 - \beta (\gamma - \gamma_{\text{ref}}), \tag{9}$$

 Table 1

 Material properties of a Li|LiCl-LiF(70:30)|Bi LMB at 550°C [31-36] (\* estimated values).

symbol	unit	Li	salt	Bi	Cu	steel	$Al_2O_3$
ν	m <sup>2</sup> /s	_	$*1.6 \cdot 10^{-6}$	$1.2 \cdot 10^{-7}$	_	_	_
ρ	kg/m <sup>3</sup>	482	1568	9721	2800	7711	3750
σ	S/m	$2.5 \cdot 10^{6}$	409	6.9·10 <sup>5</sup>	$58 \cdot 10^{6}$	*1.4.106	*0

with  $\beta$  denoting the solutal expansion coefficient,  $\gamma$  the mass concentration of Li (in kg/m<sup>3</sup>) and  $\gamma_{ref}$  the reference concentration. The velocities are coupled at the electrolyte-positive electrode interface with appropriate boundary conditions. Finally, the mass concentration of Li in Bi is determined by solving [22]

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\boldsymbol{u}\gamma) = \nabla \cdot (D\nabla\gamma). \tag{10}$$

The concentration gradient of Li at the electrolyte-positive electrode interface is given by Faraday's law as

$$\nabla \gamma \cdot \boldsymbol{n} = -\frac{jM}{zFD} \cdot \boldsymbol{n},\tag{11}$$

with the molar mass of Li M, the Faraday constant F, the interface normal vector n and the number of exchanged electrons z. The Li concentration at the electrolyte-interface is then mapped to the global mesh, and converted to molar fraction using a constant reference concentration of Bi. This is used then to compute the open-circuit potential according to eqn. (1).

The geometry is meshed with approximately 3 million purely orthogonal control volumes (180 cells over the diameter), with the positive electrode being strongly refined (30 cells over the height). The time step is chosen such that the Courant-Friedrich-Lewy condition [41] is fulfilled; specifically the CFL number is limited to 0.5. As we assume the Lorentz force and thickness of the positive electrode to be constant, we restrict the simulation time to a few minutes. All temperature effects are neglected by keeping the cell at a constant temperature of 550°C. Finally, our model does not include solidification – therefore, we will not show overpotentials in the two-phase area.

#### 3. Results & discussion

We simulate the discharge of a 10 cm diameter Li||Bi cell at a constant current of 62.2 A, which corresponds to a current density of 1 A/cm<sup>2</sup> based on the positive electrode-electrolyte interface. Firstly, we study a fully charged cell, with a homogeneous Li molar fraction of x = 0.02, and thereafter a medium charged cell with x = 0.4. The latter can be expected e.g. after a limited charge of an empty cell. Each case is simulated with and without electro-vortex flow, as well as with the influence of an artificial vertical magnetic field. A small field in the order of  $B_z = 0.05$  mT is always present from the Earth's magnetism, while larger ones up to 1 mT might readily be generated by looping the supply lines of the cells.

For a certain validation of our numerical solution, we plot in Fig. 2a also the cell potential, obtained using an analytical solution for diffusion (eqn. (6) in Ref. [22]). The latter assumes a uniform mass flux of lithium corresponding to a current density of 1 A/cm<sup>2</sup> on top of a semi-infinite positive electrode.

We clearly observe in Fig. 2 that already a simple electro-vortex flow alone may reduce the concentration overpotential by about 8 mV. The flow profile, as illustrated in Fig. 3 resembles much the one observed in Ref. [24], and can be explained by the slightly lateral current supply (see Fig. 1). Although the flow velocity is small (1 mm/s) it helps to move the Li from the centre of the cell to the outside (compare Fig. 3b and c). The vertical mixing is, however, very limited.

Vertical magnetic fields are known to generate a strong swirling flow easily [23,24,42]. We apply therefore a vertical field of 0.5 mT (i.e. 10 times the Earth magnetic field), and observe a strong rotating flow with a peak velocity of 10 mm/s (Fig. 4b). This swirl primarily pushes the Li from the centre to the rim of the cell, but mixes vertically as well, as illustrated in Fig. 4c. The concentration overpotential is reduced up to



**Fig. 2.** Cell potential (a) and concentration polarisation (b) for a fully charged LMB (x = 0.02), and the same for a medium discharged cell (x = 0.4) (c–d). The points in (a) show the cell potential using an analytical solution for pure diffusion [22]. We do not show the overpotential when the alloy solidifies in (d), because we do not use a solidification model. The discharge current density is 1 A/cm<sup>2</sup> in all cases.



**Fig. 3.** Alloy density without (b) and with flow (c), and the flow velocity (d) at the positive electrode-electrolyte interface, as well as the corresponding cross-sections of the positive electrode (a,e). The cell was fully charged (x = 0.02), the vertical magnetic field is zero and t = 5 min. (a) and (e) are stretched by a factor of three in vertical direction.

37 mV, which is much more than with a simple electro-vortex flow (Fig. 2b). Interestingly, only the onset of the flow depends much on the magnitude of the vertical field, but not the final overpotential (Fig. 2a and b).

Finally, we discharge an already fairly empty cell (Fig. 2c and d). When reaching a local Li-mole fraction of x = 0.525 the intermetallic phase is formed, and the cell potential stabilises. As we observe in Fig. 2c, it is possible to delay the formation of this solid layer considerably by applying an electro-vortex flow. This way, we might extend the capacity usage especially of Na-, K- and Ca-based liquid metal batteries in which intermetallics are a serious concern.

All results shown before were obtained for cylindrical, 10 cm diameter cells at 1 A/cm<sup>2</sup>. It can be expected that in square cells similar flows will have a similar effect; however, one might suspect that the corners are less well mixed and that Li accumulates there. Knowing that – above a certain threshold – electro-vortex flows scale linearly with the current, it is very much probable that larger batteries – with larger total cell currents – will benefit from stronger flow with better mixing. Finally, we conducted a number of simulations at 300 mA/cm<sup>2</sup>. There, we still observed a strong reduction of concentration polarisation as long as a vertical magnetic field was present. It might, however, be challenging to generate this field (in the order of 0.5 mT) by the now relatively low total cell currents alone. Given that concentration polarisation and undesirable



**Fig. 4.** Alloy density (a) and fluid flow (b) at the positive electrode-electrolyte interface and corresponding cross-section of the positive electrode (c) for a vertical magnetic field of  $B_z = 0.5$  mT. The cell was fully charged (x = 0.02) and t = 5 min. (c) is stretched by a factor of three in vertical direction.

solidification is mostly a challenge at high current densities, the combination of electro-vortex flow with a vertical magnetic field can be indeed beneficial to improve cell efficiency under realistic conditions.

#### 4. Summary

We have modelled the electric potential, current density, buoyant electro-vortex flow and Li concentration in a 10 cm diameter Li||Bi liquid metal battery (LMB). Simulating only the discharge at 1 A/cm<sup>2</sup>, we compared the effect of pure diffusive Li-transport, simple electro-vortex flow and a swirling flow in the positive electrode. We found that even electro-vortex flow alone can reduce the concentration overpotential up to 13%. Swirling flow, however, reduces the voltage losses up to 62% and is therefore still better suited to enhance mass transfer in LMBs. The magnetic field, which drives this swirling flow, might be generated e.g. by a loop in the current supply lines. Besides of reducing polarisation effects, we have shown that fluid flow delays the formation of solid intermetallic layers, as well. Overall, improved mixing increases capacity usage and prevents the potentially damaging effects of intermetallics formation.

#### Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: D. Sadoway is involved as chief scientific advisor in the company AMBRI. The other authors declare that they have no competing financial interest or personal relationships.

#### Acknowledgement

This work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) by award number 338560565, by a postdoc fellowship of the German Academic Exchange Service (DAAD) and in frame of the Helmholtz - RSF Joint Research Group "Magneto-hydrodynamic instabilities: Crucial relevance for large scale liquid metal batteries and the sun-climate connection", contract No. HRSF-0044 and RSF-18-41-06201. The computations were performed on a HPC-Cluster at the Centre for Information Services and High Performance Computing (ZIH) at TU Dresden and on the cluster "Hemera" at Helmholtz-Zentrum Dresden – Rossendorf. Fruitful discussions with S. Bénard and an anonymous referee are gratefully acknowledged.

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